

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 166 °C

Global applicability domain: Inside

Local applicability domain index: 5.12e-01

Confidence level: 3.89e-01

Nearest Neighbors from the Training Set

Image not found

Phthalide

Measured: 210

Predicted: 166

Image not found

1,2-Benzenedicarbonyl
dichloride

Measured: 15.5

Predicted: 47.5

Image not found

1,3-Benzenedicarbonyl
dichloride

Measured: 43.5

Predicted: 47.7

Image not found

1,4-Benzenedicarbonyl
dichloride

Measured: 83.5

Predicted: 47.8

Image not found

Benzenesulfonyl chloride, 2,4,6-
trimethyl-

Measured: 56.0

Predicted: 52.4